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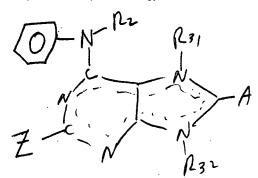
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R2=H,

Oney R31, R32 = H; other to H, G-4 alkal,

Q=H, OH, OCI-Halleye,

Point of Contact:

Mary Hale Technical Info. Specialist CM1 12D16 Tel: 308-4258

P4 = H/0/N/C

Technical Into CM1 12D167

P5 = N/0/C strate As- rings

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A= HICH3

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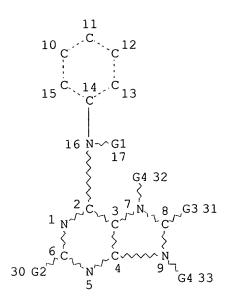
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STR



 $0 \sim Ak$ $C \sim G5 \sim G6$ 034 35 042 43 44

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Page 2-A
VAR G1=H/19
VAR G2=N/X/21/24
VAR G3=H/ME
VAR G4=H/AK/42
REP G5=(0-3) C
VAR G6=34/N/36/AK/H/OH
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 44

STEREO ATTRIBUTES: NONE
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39 ANSWERS

L6 ANSWER 1 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 204633-49-8 REGISTRY

CN 1H-Purin-6-amine, N-(4-butoxyphenyl)-2-chloro- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C15 H16 C1 N5 O

SR CA

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 128:230182 Solution-phase synthesis of 2,6,9-trisubstituted purines. Fiorini, Maria T.; Abell, Chris (University Chemical

Laboratory,
Cambridge, CB2 IEW, UK). Tetrahedron Lett., 39(13), 1827-1830 (English)
1998. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science
Ltd..

AB A simple three-step method for the soln.-phase combinatorial synthesis of 2,6,9-trisubstituted purines from 2,6-dichloropurine is described. The synthesis exploits the use of resin capture to remove excess reagent used in the final step.

L6 ANSWER 2 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 204633-45-4 REGISTRY

CN 1H-Purin-6-amine, 2-chloro-N-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C12 H10 C1 N5 O

SR CA

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 128:230182 Solution-phase synthesis of 2,6,9-trisubstituted purines. Fiorini, Maria T.; Abell, Chris (University Chemical Laboratory,

Cambridge, CB2 IEW, UK). Tetrahedron Lett., 39(13), 1827-1830 (English) 1998. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science Ltd..

AB A simple three-step method for the soln.-phase combinatorial synthesis of 2,6,9-trisubstituted purines from 2,6-dichloropurine is described. The synthesis exploits the use of resin capture to remove excess reagent used in the final step.

L6 ANSWER 3 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 204633-44-3 REGISTRY

CN 1H-Purin-6-amine, 2-chloro-N-[4-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C14 H14 C1 N5

SR CA

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 128:230182 Solution-phase synthesis of 2,6,9-trisubstituted purines. Fiorini, Maria T.; Abell, Chris (University Chemical Laboratory,

Cambridge, CB2 IEW, UK). Tetrahedron Lett., 39(13), 1827-1830 (English) 1998. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science Ltd..

AB A simple three-step method for the soln.-phase combinatorial synthesis of 2,6,9-trisubstituted purines from 2,6-dichloropurine is described. The synthesis exploits the use of resin capture to remove excess reagent used in the final step.

L6 ANSWER 4 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 204633-43-2 REGISTRY

CN 1H-Purin-6-amine, 2-chloro-N-(2,3-dihydro-1H-inden-5-yl)- (9CI) (CA INDEX

NAME)

FS 3D CONCORD

MF C14 H12 C1 N5

SR CA

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 128:230182 Solution-phase synthesis of 2,6,9-trisubstituted purines. Fiorini, Maria T.; Abell, Chris (University Chemical Laboratory,

Cambridge, CB2 IEW, UK). Tetrahedron Lett., 39(13), 1827-1830 (English) 1998. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science Ltd..

AB A simple three-step method for the soln.-phase combinatorial synthesis of 2,6,9-trisubstituted purines from 2,6-dichloropurine is described. The synthesis exploits the use of resin capture to remove excess reagent used in the final step.

L6 ANSWER 5 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 190655-08-4 REGISTRY

CN 1H-Purin-6-amine, 2-chloro-N-[4-chloro-3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C12 H6 C12 F3 N5

SR CA

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 127:34237 Preparation of purine derivatives. Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal (Novartis Ag,

Switz.; Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal). PCT Int. Appl. WO 9716452 Al 19970509, 97 pp. DESIGNATED STATES: W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP4573 19961022. PRIORITY: CH 1995-3094 19951101;

J

CH 1996-2213 19960910.

1996-2213 19960910. GI

$$\begin{array}{c|c} Rq & & \\ & & R^2m \\ & & N \\ & & N \\ & & R^2n \end{array}$$

2-Amino-6-anilino-purine derivs. I (R = halo, alkyl, HO, alkanoyloxy, alkoxy, substituted alkoxy, carboxyl, alkoxycarbonyl, carbamoyl, amino, aminosulfonyl, F3C; R1 = H, carbamoyl, alkylcarbamoyl; R2 = alkyl, Ph, substituted Ph; R3 = H, amino, phenylamino, alkylamino, HO, phenoxy, alkoxy, acyl, carbocyclic radical, or heterocyclic radical; R4 = amino, OH, phenoxy, alkoxy, acyl, substituted hydrocarbon radical, carbocyclic radical, or heterocyclic radical; R3R4 may form a ring; m and n are 0, 1; q = 1-5) were prepd. These compds. inhibit p34cdc2/cyclin Bcdc13 kinase and can be used for treatment of hyperproliferative diseases, for example tumor diseases (no data). Thus,

2-chloro-6-(3-chlorophenylamino)-9-ethyl-9H-purine, prepd. in two steps from 3-chloroaniline and 2,6-dichloropurine, was treated with ethylenediamine to give 2-(2-aminoethylamino)-6-(3-chlorophenylamino)-9-ethyl-9H-purine. L6 ANSWER 6 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 190655-06-2 REGISTRY

CN 1H-Purin-6-amine, N-[3,5-bis(trifluoromethyl)phenyl]-2-chloro- (9CI) (CF INDEX NAME)

FS 3D CONCORD

MF C13 H6 C1 F6 N5

SR CA

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 127:34237 Preparation of purine derivatives. Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal (Novartis Ag,

Switz.; Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal). PCT Int. Appl. WO 9716452 A1 19970509, 97 pp. DESIGNATED STATES: W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP4573 19961022. PRIORITY: CH 1995-3094 19951101;

CH 1996-2213 19960910.

GΙ

$$Rq$$
 NR^1
 R^2m
 R^3R^4N
 N
 R^2m
 R^2m

2-Amino-6-anilino-purine derivs. I (R = halo, alkyl, HO, alkanoyloxy, alkoxy, substituted alkoxy, carboxyl, alkoxycarbonyl, carbamoyl, amino, aminosulfonyl, F3C; R1 = H, carbamoyl, alkylcarbamoyl; R2 = alkyl, Ph, substituted Ph; R3 = H, amino, phenylamino, alkylamino, HO, phenoxy, alkoxy, acyl, carbocyclic radical, or heterocyclic radical; R4 = amino, OH, phenoxy, alkoxy, acyl, substituted hydrocarbon radical, carbocyclic

radical, or heterocyclic radical; R3R4 may form a ring; m and n are 0, 1; q=1-5) were prepd. These compds. inhibit p34cdc2/cyclin Bcdc13 kinase and can be used for treatment of hyperproliferative diseases, for example tumor diseases (no data). Thus,

2-chloro-6-(3-chlorophenylamino)-9-ethyl-

9H-purine, prepd. in two steps from 3-chloroaniline and 2,6-dichloropurine, was treated with ethylenediamine to give 2-(2-aminoethylamino)-6-(3-chlorophenylamino)-9-ethyl-9H-purine.

L6 ANSWER 7 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 190654-98-9 REGISTRY

CN 1H-Purin-6-amine, 2-chloro-N-(4-fluorophenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C11 H7 C1 F N5

SR CA

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 127:34237 Preparation of purine derivatives. Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal (Novartis Ag,

Switz.; Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal). PCT Int. Appl. WO 9716452 A1 19970509, 97 pp. DESIGNATED STATES: W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KP, KR, LC, LK, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP4573 19961022. PRIORITY: CH 1995-3094 19951101;

CH 1996-2213 19960910.

$$Rq$$
 NR^1
 R^2m
 R^3R^4N
 R^2n
 R^2n

AB 2-Amino-6-anilino-purine derivs. I (R = halo, alkyl, HO, alkanoyloxy, alkoxy, substituted alkoxy, carboxyl, alkoxycarbonyl, carbamoyl, amino, aminosulfonyl, F3C; R1 = H, carbamoyl, alkylcarbamoyl; R2 = alkyl, Ph, substituted Ph; R3 = H, amino, phenylamino, alkylamino, HO, phenoxy, alkoxy, acyl, carbocyclic radical, or heterocyclic radical; R4 = amino, OH, phenoxy, alkoxy, acyl, substituted hydrocarbon radical, carbocyclic radical, or heterocyclic radical; R3R4 may form a ring; m and n are 0, 1; q = 1-5) were prepd. These compds. inhibit p34cdc2/cyclin Bcdc13 kinase and can be used for treatment of hyperproliferative diseases, for example tumor diseases (no data). Thus,

2-chloro-6-(3-chlorophenylamino)-9-ethyl-

9H-purine, prepd. in two steps from 3-chloroaniline and 2,6-dichloropurine, was treated with ethylenediamine to give 2-(2-aminoethylamino)-6-(3-chlorophenylamino)-9-ethyl-9H-purine.

L6 ANSWER 8 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 190654-96-7 REGISTRY

CN Benzonitrile, 3-[(2-chloro-1H-purin-6-yl)amino]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C12 H7 C1 N6

SR CA

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 127:34237 Preparation of purine derivatives. Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal (Novartis Ag,

Switz.; Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal). PCT Int. Appl. WO 9716452 Al 19970509, 97 pp. DESIGNATED STATES: W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT,

BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP4573 19961022. PRIORITY: CH 1995-3094 19951101;

CH 1996-2213 19960910.

GΙ

$$R_q$$
 NR^1
 R^2m
 R^3R^4N
 R^2n
 R^2n

2-Amino-6-anilino-purine derivs. I (R = halo, alkyl, HO, alkanoyloxy, alkoxy, substituted alkoxy, carboxyl, alkoxycarbonyl, carbamoyl, amino, aminosulfonyl, F3C; R1 = H, carbamoyl, alkylcarbamoyl; R2 = alkyl, Ph, substituted Ph; R3 = H, amino, phenylamino, alkylamino, HO, phenoxy, alkoxy, acyl, carbocyclic radical, or heterocyclic radical; R4 = amino, OH, phenoxy, alkoxy, acyl, substituted hydrocarbon radical, carbocyclic radical, or heterocyclic radical; R3R4 may form a ring; m and n are 0, 1; q = 1-5) were prepd. These compds. inhibit p34cdc2/cyclin Bcdc13 kinase and can be used for treatment of hyperproliferative diseases, for example tumor diseases (no data). Thus,

2-chloro-6-(3-chlorophenylamino)-9-ethyl-

9H-purine, prepd. in two steps from 3-chloroaniline and 2,6-dichloropurine, was treated with ethylenediamine to give 2-(2-aminoethylamino)-6-(3-chlorophenylamino)-9-ethyl-9H-purine.

L6 ANSWER 9 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 190654-94-5 REGISTRY

CN 1H-Purin-6-amine, 2-chloro-N-(3-fluorophenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C11 H7 C1 F N5

SR CA

LC STN Files: CA, CAPLUS

2 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 128:230182 Solution-phase synthesis of 2,6,9-trisubstituted

purines. Fiorini, Maria T.; Abell, Chris (University Chemical Laboratory,

Cambridge, CB2 IEW, UK). Tetrahedron Lett., 39(13), 1827-1830 (English) 1998. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science

Ltd..

AB A simple three-step method for the soln.-phase combinatorial synthesis of 2,6,9-trisubstituted purines from 2,6-dichloropurine is described. The synthesis exploits the use of resin capture to remove excess reagent used in the final step.

REFERENCE 2: 127:34237 Preparation of purine derivatives. Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal (Novartis

Αg,

Switz.; Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal). PCT Int. Appl. WO 9716452 A1 19970509, 97 pp. DESIGNATED STATES: W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP4573 19961022. PRIORITY: CH 1995-3094 19951101;

CH

1996-2213 19960910.

GΙ

$$Rq$$
 NR^1
 R^2m
 R^3R^4N
 R^2n
 R^2n

2-Amino-6-anilino-purine derivs. I (R = halo, alkyl, HO, alkanoyloxy, alkoxy, substituted alkoxy, carboxyl, alkoxycarbonyl, carbamoyl, amino, aminosulfonyl, F3C; R1 = H, carbamoyl, alkylcarbamoyl; R2 = alkyl, Ph, substituted Ph; R3 = H, amino, phenylamino, alkylamino, HO, phenoxy, alkoxy, acyl, carbocyclic radical, or heterocyclic radical; R4 = amino, OH, phenoxy, alkoxy, acyl, substituted hydrocarbon radical, carbocyclic radical, or heterocyclic radical; R3R4 may form a ring; m and n are 0, 1; q = 1-5) were prepd. These compds. inhibit p34cdc2/cyclin Bcdc13 kinase and can be used for treatment of hyperproliferative diseases, for example tumor diseases (no data). Thus,

2-chloro-6-(3-chlorophenylamino)-9-ethyl-

9H-purine, prepd. in two steps from 3-chloroaniline and 2,6-dichloropurine, was treated with ethylenediamine to give 2-(2-aminoethylamino)-6-(3-chlorophenylamino)-9-ethyl-9H-purine.

- L6 ANSWER 10 OF 39 REGISTRY COPYRIGHT 2000 ACS
- RN 190654-92-3 REGISTRY
- CN 1H-Purin-6-amine, 2-chloro-N-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)
- FS 3D CONCORD
- MF C14 H14 C1 N5 O3
- SR CA
- LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 127:34237 Preparation of purine derivatives. Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal (Novartis Ag,

Switz.; Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal). PCT Int. Appl. WO 9716452 Al 19970509, 97 pp. DESIGNATED STATES: W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP4573 19961022. PRIORITY: CH 1995-3094 19951101;

CH 1996-2213 19960910.

GI

$$Rq$$
 NR^{1}
 $R^{2}m$
 N
 N
 $R^{2}n$
 $R^{2}n$
 $R^{2}n$

AB 2-Amino-6-anilino-purine derivs. I (R = halo, alkyl, HO, alkanoyloxy, alkoxy, substituted alkoxy, carboxyl, alkoxycarbonyl, carbamoyl, amino, aminosulfonyl, F3C; R1 = H, carbamoyl, alkylcarbamoyl; R2 = alkyl, Ph, substituted Ph; R3 = H, amino, phenylamino, alkylamino, HO, phenoxy, alkoxy, acyl, carbocyclic radical, or heterocyclic radical; R4 = amino, OH, phenoxy, alkoxy, acyl, substituted hydrocarbon radical, carbocyclic radical, or heterocyclic radical; R3R4 may form a ring; m and n are 0, 1; q = 1-5) were prepd. These compds. inhibit p34cdc2/cyclin Bcdc13 kinase and can be used for treatment of hyperproliferative diseases, for example tumor diseases (no data). Thus,

2-chloro-6-(3-chlorophenylamino)-9-ethyl-9H-purine, prepd. in two steps from 3-chloroaniline and 2,6-dichloropurine, was treated with ethylenediamine to give 2-(2-aminoethylamino)-6-(3-chlorophenylamino)-9-ethyl-9H-purine.

CN 1-Propanol, 3-[[6-[(3-methoxyphenyl)amino]-1H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C15 H18 N6 O2

SR CA

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 127:34237 Preparation of purine derivatives. Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal (Novartis Ag,

Switz.; Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal). PCT Int. Appl. WO 9716452 Al 19970509, 97 pp. DESIGNATED STATES: W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP4573 19961022. PRIORITY: CH 1995-3094 19951101;

CH

1996-2213 19960910.

GI

$$R_{q}$$
 NR^{1}
 R^{2}_{m}
 N
 R^{2}_{n}
 R^{2}_{n}
 R^{2}_{n}

AB 2-Amino-6-anilino-purine derivs. I (R = halo, alkyl, HO, alkanoyloxy, alkoxy, substituted alkoxy, carboxyl, alkoxycarbonyl, carbamoyl, amino, aminosulfonyl, F3C; R1 = H, carbamoyl, alkylcarbamoyl; R2 = alkyl, Ph, substituted Ph; R3 = H, amino, phenylamino, alkylamino, HO, phenoxy, alkoxy, acyl, carbocyclic radical, or heterocyclic radical; R4 = amino,

OH, phenoxy, alkoxy, acyl, substituted hydrocarbon radical, carbocyclic radical, or heterocyclic radical; R3R4 may form a ring; m and n are 0, 1; q=1-5) were prepd. These compds. inhibit p34cdc2/cyclin Bcdc13 kinase and can be used for treatment of hyperproliferative diseases, for example tumor diseases (no data). Thus,

2-chloro-6-(3-chlorophenylamino)-9-ethyl-

9H-purine, prepd. in two steps from 3-chloroaniline and 2,6-dichloropurine, was treated with ethylenediamine to give 2-(2-aminoethylamino)-6-(3-chlorophenylamino)-9-ethyl-9H-purine.

L6 ANSWER 12 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 190654-89-8 REGISTRY

CN 1H-Purin-6-amine, 2-chloro-N-(3-methoxyphenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C12 H10 C1 N5 O

SR CA

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 127:34237 Preparation of purine derivatives. Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal (Novartis Ag,

Switz.; Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal). PCT Int. Appl. WO 9716452 Al 19970509, 97 pp. DESIGNATED STATES: W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KP, KR, LC, LK, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP4573 19961022. PRIORITY: CH 1995-3094 19951101;

СН

1996-2213 19960910.

$$R_q$$
 NR^1
 R^2m
 N
 R^3R^4N
 R^2n
 R^2n

AB 2-Amino-6-anilino-purine derivs. I (R = halo, alkyl, HO, alkanoyloxy, alkoxy, substituted alkoxy, carboxyl, alkoxycarbonyl, carbamoyl, amino, aminosulfonyl, F3C; R1 = H, carbamoyl, alkylcarbamoyl; R2 = alkyl, Ph, substituted Ph; R3 = H, amino, phenylamino, alkylamino, HO, phenoxy, alkoxy, acyl, carbocyclic radical, or heterocyclic radical; R4 = amino, OH, phenoxy, alkoxy, acyl, substituted hydrocarbon radical, carbocyclic radical, or heterocyclic radical; R3R4 may form a ring; m and n are 0, 1; q = 1-5) were prepd. These compds. inhibit p34cdc2/cyclin Bcdc13 kinase and can be used for treatment of hyperproliferative diseases, for example tumor diseases (no data). Thus,

2-chloro-6-(3-chlorophenylamino)-9-ethyl-

9H-purine, prepd. in two steps from 3-chloroaniline and 2,6-dichloropurine, was treated with ethylenediamine to give 2-(2-aminoethylamino)-6-(3-chlorophenylamino)-9-ethyl-9H-purine.

L6 ANSWER 13 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 190654-88-7 REGISTRY

CN Benzoic acid, 3-[(2-chloro-1H-purin-6-yl)amino]-2-methyl-, ethyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C15 H14 C1 N5 O2

SR CA

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 127:34237 Preparation of purine derivatives. Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal (Novartis Ag,

Switz.; Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal). PCT Int. Appl. WO 9716452 Al 19970509, 97 pp. DESIGNATED STATES: W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP4573 19961022. PRIORITY: CH 1995-3094 19951101;

СН

1996-2213 19960910.

GI

$$Rq$$
 NR^1
 R^2m
 N
 R^3R^4N
 N
 R^2n
 R^2n

AB 2-Amino-6-anilino-purine derivs. I (R = halo, alkyl, HO, alkanoyloxy, alkoxy, substituted alkoxy, carboxyl, alkoxycarbonyl, carbamoyl, amino, aminosulfonyl, F3C; R1 = H, carbamoyl, alkylcarbamoyl; R2 = alkyl, Ph, substituted Ph; R3 = H, amino, phenylamino, alkylamino, HO, phenoxy, alkoxy, acyl, carbocyclic radical, or heterocyclic radical; R4 = amino, OH, phenoxy, alkoxy, acyl, substituted hydrocarbon radical, carbocyclic radical, or heterocyclic radical; R3R4 may form a ring; m and n are 0, 1; q = 1-5) were prepd. These compds. inhibit p34cdc2/cyclin Bcdc13 kinase and can be used for treatment of hyperproliferative diseases, for example tumor diseases (no data). Thus,

2-chloro-6-(3-chlorophenylamino)-9-ethyl-

9H-purine, prepd. in two steps from 3-chloroaniline and 2,6-dichloropurine, was treated with ethylenediamine to give 2-(2-aminoethylamino)-6-(3-chlorophenylamino)-9-ethyl-9H-purine.

L6 ANSWER 14 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 190654-85-4 REGISTRY

CN 1H-Purin-6-amine, 2-chloro-N-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX

NAME)

FS 3D CONCORD

MF C12 H7 C1 F3 N5

SR CA

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 127:34237 Preparation of purine derivatives. Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal (Novartis Ag,

Switz.; Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal). PCT Int. Appl. WO 9716452 A1 19970509, 97 pp. DESIGNATED STATES: W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI,

SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP4573 19961022. PRIORITY: CH 1995-3094 19951101;

СН

1996-2213 19960910.

GΙ

$$Rq$$
 $NR1$
 $R^{2}m$
 N
 N
 N
 $R^{2}n$
 N

2-Amino-6-anilino-purine derivs. I (R = halo, alkyl, HO, alkanoyloxy, alkoxy, substituted alkoxy, carboxyl, alkoxycarbonyl, carbamoyl, amino, aminosulfonyl, F3C; R1 = H, carbamoyl, alkylcarbamoyl; R2 = alkyl, Ph, substituted Ph; R3 = H, amino, phenylamino, alkylamino, HO, phenoxy, alkoxy, acyl, carbocyclic radical, or heterocyclic radical; R4 = amino, OH, phenoxy, alkoxy, acyl, substituted hydrocarbon radical, carbocyclic radical, or heterocyclic radical; R3R4 may form a ring; m and n are 0, 1; q = 1-5) were prepd. These compds. inhibit p34cdc2/cyclin Bcdc13 kinase and can be used for treatment of hyperproliferative diseases, for example tumor diseases (no data). Thus,

2-chloro-6-(3-chlorophenylamino)-9-ethyl-

9H-purine, prepd. in two steps from 3-chloroaniline and 2,6-dichloropurine, was treated with ethylenediamine to give 2-(2-aminoethylamino)-6-(3-chlorophenylamino)-9-ethyl-9H-purine.

L6 ANSWER 15 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 190654-76-3 REGISTRY

CN 1H-Purin-6-amine, 2-chloro-N-(3-chlorophenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C11 H7 C12 N5

SR CA

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 127:34237 Preparation of purine derivatives. Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal (Novartis Aq,

Switz.; Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal). PCT Int. Appl. WO 9716452 Al 19970509, 97 pp. DESIGNATED STATES: W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP4573 19961022. PRIORITY: CH 1995-3094 19951101;

CH 1996-2213 19960910.

GΙ

$$Rq$$

$$NR^{1}$$

$$R^{2}m$$

$$N$$

$$R^{2}n$$

2-Amino-6-anilino-purine derivs. I (R = halo, alkyl, HO, alkanoyloxy, alkoxy, substituted alkoxy, carboxyl, alkoxycarbonyl, carbamoyl, amino, aminosulfonyl, F3C; R1 = H, carbamoyl, alkylcarbamoyl; R2 = alkyl, Ph, substituted Ph; R3 = H, amino, phenylamino, alkylamino, HO, phenoxy, alkoxy, acyl, carbocyclic radical, or heterocyclic radical; R4 = amino, OH, phenoxy, alkoxy, acyl, substituted hydrocarbon radical, carbocyclic radical, or heterocyclic radical; R3R4 may form a ring; m and n are 0, 1; q = 1-5) were prepd. These compds. inhibit p34cdc2/cyclin Bcdc13 kinase and can be used for treatment of hyperproliferative diseases, for example tumor diseases (no data). Thus,

2-chloro-6-(3-chlorophenylamino)-9-ethyl-

9H-purine, prepd. in two steps from 3-chloroaniline and 2,6-dichloropurine, was treated with ethylenediamine to give 2-(2-aminoethylamino)-6-(3-chlorophenylamino)-9-ethyl-9H-purine.

L6 ANSWER 16 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 185409-07-8 REGISTRY

CN Ethanol, 2-[[6-(phenylamino)-1H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C13 H14 N6 O

SR CA

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:74664 Facile Preparation of 2,6-Disubstituted Purines Using

Solid-Phase Chemistry. Nugiel, David A.; Cornelius, Lyndon A. M.; Corbett, Jeffrey W. (DuPont Merck Pharmaceutical Company, Wilmington, DE, 19880-0500, USA). J. Org. Chem., 62(1), 201-203 (English) 1997. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

AB A solid-phase approach to the prepn. of novel 2,6-disubstituted purines is

presented. 2,6-Dichloropurine was loaded onto a THP linked solid support through the N-9 nitrogen. Displacement of the 6-chloro position was accomplished using excess amine at 80.degree. in n-butanol. The 2-chloro position required more forcing conditions and was displaced using an

as solvent at 150 .degree.C. The final products were cleaved from the resin to give the desired targets in 85-95% crude yield. Various primary and secondary amines, anilines and sulfonamides could be introduced at

6-position of purine and subsequently modified at the 2-position. This approach was used to prep. olomoucine, a selective p33cdk2/cyclin A inhibitor, in three steps and 60% overall yield.

L6 ANSWER 17 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 185408-97-3 REGISTRY

CN 1H-Purin-6-amine, 2-chloro-N-phenyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C11 H8 C1 N5

SR CA

the

the

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:74664 Facile Preparation of 2,6-Disubstituted Purines Using

Solid-Phase Chemistry. Nugiel, David A.; Cornelius, Lyndon A. M.; Corbett, Jeffrey W. (DuPont Merck Pharmaceutical Company, Wilmington, DE, 19880-0500, USA). J. Org. Chem., 62(1), 201-203 (English) 1997. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

AB A solid-phase approach to the prepn. of novel 2,6-disubstituted purines is

presented. 2,6-Dichloropurine was loaded onto a THP linked solid support through the N-9 nitrogen. Displacement of the 6-chloro position was accomplished using excess amine at 80.degree. in n-butanol. The 2-chloro position required more forcing conditions and was displaced using an amine

as solvent at 150 .degree.C. The final products were cleaved from the resin to give the desired targets in 85-95% crude yield. Various primary and secondary amines, anilines and sulfonamides could be introduced at

6-position of purine and subsequently modified at the 2-position. This

approach was used to prep. olomoucine, a selective p33cdk2/cyclin A inhibitor, in three steps and 60% overall yield.

L6 ANSWER 18 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 151644-04-1 REGISTRY

CN 1H-Purine-2,6-diamine, N6-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C12 H12 N6 O

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:29465 Preparation of (2',3'-dideoxy-3'-.beta.-D-erythropentofuranosyl)-9H-purines as antiviral nucleosides. Burns, Charlene Louise; Koszalka, George Walter; Krenitsky, Thomas Anthony (Wellcome Foundation Ltd., UK). PCT Int. Appl. WO 9314103 Al 19930722, 94

pp. DESIGNATED STATES: RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1993-GB4 19930105. PRIORITY: GB 1992-149 19920106; GB 1992-20317 19920925.

GΙ

AB Title compds. I [R1 = H, amino, halo; R2 = halo; NR4R5, R4, R5 = H, C1-4 hydroxyalkyl, C1-6 alkyl, C3-6 cycloalkyl, C2-6 alkenyl, C6-10 aryl, (un)substituted C6-10arylC1-3alkyl, etc.; R6O(Ar)(CH2)n (R6 = C1-6 alkyl, Ar = C6-10 aryl, n = 0-3); R4R5 = N of a 3 to 7-membered heterocyclic ring

optionally contg. 1 or more other hetero atoms selected from O, N, S; S(O)nR7, n = 0-2, R7 = C1-6 alkyl, C3-6 cycloalkyl, etc.; OR8, R8 = H, C1-6 alkyl, C3-6 cycloalkyl, etc.; R3 = H, amino, halo, C1-6 alkyl with proviso] were prepd. as antiviral nucleosides. Thus, 2-amino-6-dimethylamino-9H-purine and 2',3'-dideoxy-3'-fluorouridine were suspended in a potassium phosphate buffer contg. potassium azide and treated with purine nucleoside phosphorylase and thymidine phosphorylase immobilized

on

DEAE cellulose to give 26% I (R1 = NH2, R2 = Me2N, R3 = H) (II). II showed an IC50 = 8.mu.M against HIV in MT4 cells. Various formulations for I are also reported.

L6 ANSWER 19 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 120045-95-6 REGISTRY

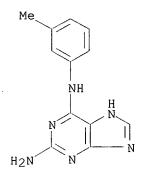
CN 1H-Purine-2,6-diamine, N6-(3-methylphenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C12 H12 N6

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT (*File contains numerically searchable property data)



no util

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:217083 The mass spectrometry of 2-amino-6-arylaminopurines.

Yakout, E. M. A. (Dep. Pesticide Chem., Natl. Res. Cent., Cairo, Egypt). Bull. Natl. Res. Cent. (Egypt), 18(1), 11-17 (English) 1993. CODEN: BNRCET.

AB Principal modes of fragmentation of the title spectra under electron impact were detd.

REFERENCE 2: 110:172972 Phosphorus pentoxide in organic synthesis. XXXVII. Synthesis of 2-amino-6-arylaminopurines. Yakout, El Sayed M. A.; Soe, Henrik M.; Pedersen, Erik B. (Dep. Chem., Odense Univ., Odense, DK-5230, Den.). Acta Chem. Scand., Ser. B, B42(4), 257-8 (English) 1988. CODEN: ACBOCV. ISSN: 0302-4369.

L6 ANSWER 20 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 120045-94-5 REGISTRY

CN 1H-Purine-2,6-diamine, N6-(3-fluorophenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C11 H9 F N6

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT (*File contains numerically searchable property data)

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:217083 The mass spectrometry of 2-amino-6-arylaminopurines.

Yakout, E. M. A. (Dep. Pesticide Chem., Natl. Res. Cent., Cairo, Egypt). Bull. Natl. Res. Cent. (Egypt), 18(1), 11-17 (English) 1993. CODEN: BNRCET.

AB Principal modes of fragmentation of the title spectra under electron impact were detd.

REFERENCE 2: 110:172972 Phosphorus pentoxide in organic synthesis. XXXVII. Synthesis of 2-amino-6-arylaminopurines. Yakout, El Sayed M. A.; Soe, Henrik M.; Pedersen, Erik B. (Dep. Chem., Odense Univ., Odense, DK-5230, Den.). Acta Chem. Scand., Ser. B, B42(4), 257-8 (English) 1988. CODEN: ACBOCV. ISSN: 0302-4369.

L6 ANSWER 21 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 120045-93-4 REGISTRY

CN 1H-Purine-2,6-diamine, N6-(3,5-dichlorophenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C11 H8 C12 N6

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT (*File contains numerically searchable property data)

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:217083 The mass spectrometry of 2-amino-6-arylaminopurines.

Yakout, E. M. A. (Dep. Pesticide Chem., Natl. Res. Cent., Cairo, Egypt). Bull. Natl. Res. Cent. (Egypt), 18(1), 11-17 (English) 1993. CODEN: BNRCET.

AB Principal modes of fragmentation of the title spectra under electron impact were detd.

REFERENCE 2: 110:172972 Phosphorus pentoxide in organic synthesis. XXXVII. Synthesis of 2-amino-6-arylaminopurines. Yakout, El Sayed M. A.; Soe, Henrik M.; Pedersen, Erik B. (Dep. Chem., Odense Univ., Odense, DK-5230, Den.). Acta Chem. Scand., Ser. B, B42(4), 257-8 (English) 1988. CODEN: ACBOCV. ISSN: 0302-4369.

L6 ANSWER 22 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 120045-92-3 REGISTRY

CN 1H-Purine-2,6-diamine, N6-(4-chlorophenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C11 H9 C1 N6

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT

(*File contains numerically searchable property data)

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:217083 The mass spectrometry of 2-amino-6-arylaminopurines.

Yakout, E. M. A. (Dep. Pesticide Chem., Natl. Res. Cent., Cairo, Egypt). Bull. Natl. Res. Cent. (Egypt), 18(1), 11-17 (English) 1993. CODEN: BNRCET.

AB Principal modes of fragmentation of the title spectra under electron impact were detd.

REFERENCE 2: 110:172972 Phosphorus pentoxide in organic synthesis. XXXVII. Synthesis of 2-amino-6-arylaminopurines. Yakout, El Sayed M. A.; Soe, Henrik M.; Pedersen, Erik B. (Dep. Chem., Odense Univ., Odense, DK-5230, Den.). Acta Chem. Scand., Ser. B, B42(4), 257-8 (English) 1988. CODEN: ACBOCV. ISSN: 0302-4369.

L6 ANSWER 23 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 120045-91-2 REGISTRY

CN 1H-Purine-2,6-diamine, N6-(4-fluorophenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C11 H9 F N6

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT (*File contains numerically searchable property data)

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:217083 The mass spectrometry of 2-amino-6-arylaminopurines.

Yakout, E. M. A. (Dep. Pesticide Chem., Natl. Res. Cent., Cairo, Egypt). Bull. Natl. Res. Cent. (Egypt), 18(1), 11-17 (English) 1993. CODEN: BNRCET.

AB Principal modes of fragmentation of the title spectra under electron impact were detd.

REFERENCE 2: 110:172972 Phosphorus pentoxide in organic synthesis. XXXVII. Synthesis of 2-amino-6-arylaminopurines. Yakout, El Sayed M. A.; Soe, Henrik M.; Pedersen, Erik B. (Dep. Chem., Odense Univ., Odense, DK-5230, Den.). Acta Chem. Scand., Ser. B, B42(4), 257-8 (English) 1988. CODEN: ACBOCV. ISSN: 0302-4369.

L6 ANSWER 24 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 120045-90-1 REGISTRY

CN 1H-Purine-2,6-diamine, N6-(4-bromophenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C11 H9 Br N6

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT (*File contains numerically searchable property data)

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:217083 The mass spectrometry of 2-amino-6-arylaminopurines.

Yakout, E. M. A. (Dep. Pesticide Chem., Natl. Res. Cent., Cairo, Egypt). Bull. Natl. Res. Cent. (Egypt), 18(1), 11-17 (English) 1993. CODEN: BNRCET.

AB Principal modes of fragmentation of the title spectra under electron impact were detd.

REFERENCE 2: 110:172972 Phosphorus pentoxide in organic synthesis. XXXVII. Synthesis of 2-amino-6-arylaminopurines. Yakout, El Sayed M. A.; Soe, Henrik M.; Pedersen, Erik B. (Dep. Chem., Odense Univ., Odense, DK-5230, Den.). Acta Chem. Scand., Ser. B, B42(4), 257-8 (English) 1988. CODEN: ACBOCV. ISSN: 0302-4369.

L6 ANSWER 25 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 120045-89-8 REGISTRY

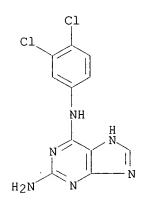
CN 1H-Purine-2,6-diamine, N6-(3,4-dichlorophenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C11 H8 C12 N6

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT (*File contains numerically searchable property data)



2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:217083 The mass spectrometry of 2-amino-6-arylaminopurines.

Yakout, E. M. A. (Dep. Pesticide Chem., Natl. Res. Cent., Cairo, Egypt). Bull. Natl. Res. Cent. (Egypt), 18(1), 11-17 (English) 1993. CODEN: BNRCET.

AB Principal modes of fragmentation of the title spectra under electron impact were detd.

REFERENCE 2: 110:172972 Phosphorus pentoxide in organic synthesis. XXXVII. Synthesis of 2-amino-6-arylaminopurines. Yakout, El Sayed M. A.; Soe, Henrik M.; Pedersen, Erik B. (Dep. Chem., Odense Univ., Odense, DK-5230, Den.). Acta Chem. Scand., Ser. B, B42(4), 257-8 (English) 1988. CODEN: ACBOCV. ISSN: 0302-4369.

L6 ANSWER 26 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 120045-88-7 REGISTRY

CN 1H-Purine-2, 6-diamine, N6-(3-chlorophenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C11 H9 C1 N6

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT

(*File contains numerically searchable property data)

No util

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 110:172972 Phosphorus pentoxide in organic synthesis. XXXVII. Synthesis of 2-amino-6-arylaminopurines. Yakout, El Sayed M. A.; Soe, Henrik M.; Pedersen, Erik B. (Dep. Chem., Odense Univ., Odense, DK-5230, Den.). Acta Chem. Scand., Ser. B, B42(4), 257-8 (English) 1988. CODEN: ACBOCV. ISSN: 0302-4369.

AB Aminopurines I (R = Ph, substituted Ph) were obtained in 45-90% yield by heating guanine with RNH2.HCl in the presence of P2O5 and Et3N.HCl.

L6 ANSWER 27 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 120045-87-6 REGISTRY

CN 1H-Purine-2,6-diamine, N6-(4-chloro-2-methylphenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C12 H11 C1 N6

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT

(*File contains numerically searchable property data)

2 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:217083 The mass spectrometry of 2-amino-6-arylaminopurines.

Yakout, E. M. A. (Dep. Pesticide Chem., Natl. Res. Cent., Cairo, Egypt). Bull. Natl. Res. Cent. (Egypt), 18(1), 11-17 (English) 1993. CODEN: BNRCET.

AB Principal modes of fragmentation of the title spectra under electron impact were detd.

REFERENCE. 2: 110:172972 Phosphorus pentoxide in organic synthesis. XXXVII. Synthesis of 2-amino-6-arylaminopurines. Yakout, El Sayed M. A.; Soe, Henrik M.; Pedersen, Erik B. (Dep. Chem., Odense Univ., Odense, DK-5230, Den.). Acta Chem. Scand., Ser. B, B42(4), 257-8 (English) 1988. CODEN: ACBOCV. ISSN: 0302-4369.

GΙ

AB Aminopurines I (R = Ph, substituted Ph) were obtained in 45-90% yield by heating guanine with RNH2.HCl in the presence of P2O5 and Et3N.HCl.

L6 ANSWER 28 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 120045-86-5 REGISTRY

CN 1H-Purine-2,6-diamine, N6-(3,5-dimethylphenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD MF C13 H14 N6

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT (*File contains numerically searchable property data)

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:217083 The mass spectrometry of 2-amino-6-arylaminopurines.

Yakout, E. M. A. (Dep. Pesticide Chem., Natl. Res. Cent., Cairo, Egypt). Bull. Natl. Res. Cent. (Egypt), 18(1), 11-17 (English) 1993. CODEN: BNRCET.

AB Principal modes of fragmentation of the title spectra under electron impact were detd.

REFERENCE 2: 110:172972 Phosphorus pentoxide in organic synthesis. XXXVII. Synthesis of 2-amino-6-arylaminopurines. Yakout, El Sayed M. A.; Soe, Henrik M.; Pedersen, Erik B. (Dep. Chem., Odense Univ., Odense, DK-5230, Den.). Acta Chem. Scand., Ser. B, B42(4), 257-8 (English) 1988. CODEN: ACBOCV. ISSN: 0302-4369.

GΙ

AB Aminopurines I (R = Ph, substituted Ph) were obtained in 45-90% yield by heating guanine with RNH2.HCl in the presence of P2O5 and Et3N.HCl.

L6 ANSWER 29 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 120045-85-4 REGISTRY

CN 1H-Purine-2,6-diamine, N6-(4-ethylphenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C13 H14 N6

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT (*File contains numerically searchable property data)

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:217083 The mass spectrometry of

2-amino-6-arylaminopurines.

Yakout, E. M. A. (Dep. Pesticide Chem., Natl. Res. Cent., Cairo, Egypt). Bull. Natl. Res. Cent. (Egypt), 18(1), 11-17 (English) 1993. CODEN: BNRCET.

AB Principal modes of fragmentation of the title spectra under electron impact were detd.

REFERENCE 2: 110:172972 Phosphorus pentoxide in organic synthesis. XXXVII. Synthesis of 2-amino-6-arylaminopurines. Yakout, El Sayed M. A.; Soe, Henrik M.; Pedersen, Erik B. (Dep. Chem., Odense Univ., Odense, DK-5230, Den.). Acta Chem. Scand., Ser. B, B42(4), 257-8 (English) 1988. CODEN: ACBOCV. ISSN: 0302-4369.

GΙ

AB Aminopurines I (R = Ph, substituted Ph) were obtained in 45-90% yield by heating guanine with RNH2.HCl in the presence of P2O5 and Et3N.HCl.

L6 ANSWER 30 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 120045-84-3 REGISTRY

CN 1H-Purine-2,6-diamine, N6-(3,4-dimethylphenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C13 H14 N6

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT (*File contains numerically searchable property data)

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:217083 The mass spectrometry of 2-amino-6-arylaminopurines.

Yakout, E. M. A. (Dep. Pesticide Chem., Natl. Res. Cent., Cairo, Egypt). Bull. Natl. Res. Cent. (Egypt), 18(1), 11-17 (English) 1993. CODEN: BNRCET.

AB Principal modes of fragmentation of the title spectra under electron impact were detd.

REFERENCE 2: 110:172972 Phosphorus pentoxide in organic synthesis. XXXVII. Synthesis of 2-amino-6-arylaminopurines. Yakout, El Sayed M. A.; Soe, Henrik M.; Pedersen, Erik B. (Dep. Chem., Odense Univ., Odense, DK-5230, Den.). Acta Chem. Scand., Ser. B, B42(4), 257-8 (English) 1988. CODEN: ACBOCV. ISSN: 0302-4369.

GΙ

AB Aminopurines I (R = Ph, substituted Ph) were obtained in 45-90% yield by heating guanine with RNH2.HCl in the presence of P2O5 and Et3N.HCl.

L6 ANSWER 31 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 52819-68-8 REGISTRY

CN 1H-Purine-2,6-diamine, N,N'-diphenyl- (9CI) (CA INDEX NAME) OTHER NAMES:

CN 2,6-Dibenzeneaminopurine

FS 3D CONCORD

MF C17 H14 N6

LC STN Files: CA, CAPLUS, TOXLIT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 81:163864 Analogs of purine bases and purine metabolism in Actinomyces olivaceus. Matselyukh, B. P.; Tkachuk, Z. Yu.; Tret'yakova, G. S.; Nedel'kina, N. N. (Inst. Microbiol. Virol, Kiev, USSR). Mikrobiol.

Zh. (Kiev), 36(3), 355-7 (Ukranian) 1974. CODEN: MZUKAV.

When added to the incubation medium at 0.1 mg/ml, 6-mercaptopurine (I) [50-44-2], 2-mercaptoadenine [3647-48-1], 8-azaguanine [134-58-7], or 2,6-dichloropurine [5451-40-1] inhibited, whereas 6-N-acetylaminopurine [6034-68-0], 6-N-benzeneaminopurine [1210-66-8], 2,6-dibenzeneaminopurine [52819-68-8], 6-N-furfurylaminopurine [525-79-1], or 2-chloro-6-purinecarboxylic acid Et ester [52819-69-9] enhanced the growth of the A. olivaceus prototrophic strain. I was an active retroinhibitor of purine nucleotide synthesis in this strain. Purine-dependent mutants of A. olivaceus did not utilize the purine analogs.

L6 ANSWER 32 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 39639-56-0 REGISTRY

CN 1H-Purine-2,6-diamine, N,N'-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C19 H18 N6

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 78:16123 Synthesis and study of 2,6-diaminopurines. Tret'yakova, G. S.; Nedel'kina, N. N.; Cherkasov, V. M. (Inst. Org. Khim.,

Kiev, USSR). Ukr. Khim. Zh. (Russ. Ed.), 38(6), 602-5 (Russian) 1972. CODEN: UKZHAU.

AB 2,6-Dichloropurine was treated with cyclohexyl-, admantyl-, and

benzylamines, and with morpholine, p-toluidine, and p-nitroaniline to replace the Cl atom in position 2. By use of more amine, disubstituted compds. were obtained using morpholine, benzylamine, and p-toluidine.

The

Cl atom of 6-chloro-2-benzylaminopurine was replaced by p-XC6H4NH (X =

Me,

NO2) and the Cl of 6-chloro-2-cyclohexylaminopurine was replaced with p-O2NC6H4NH. These compds. were prepd. as substances with possible cytokinin activity.

L6 ANSWER 33 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 39639-53-7 REGISTRY

CN 1H-Purine-2,6-diamine, N6-(4-methylphenyl)-N2-(phenylmethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C19 H18 N6

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 78:16123 Synthesis and study of 2,6-diaminopurines. Tret'yakova, G. S.; Nedel'kina, N. N.; Cherkasov, V. M. (Inst. Org. Khim.,

Kiev, USSR). Ukr. Khim. Zh. (Russ. Ed.), 38(6), 602-5 (Russian) 1972. CODEN: UKZHAU.

AB 2,6-Dichloropurine was treated with cyclohexyl-, admantyl-, and benzylamines, and with morpholine, p-toluidine, and p-nitroaniline to replace the Cl atom in position 2. By use of more amine, disubstituted compds. were obtained using morpholine, benzylamine, and p-toluidine.

The Cl atom of 6-chloro-2-benzylaminopurine was replaced by p-XC6H4NH (X = Me,

NO2) and the Cl of 6-chloro-2-cyclohexylaminopurine was replaced with p-O2NC6H4NH. These compds. were prepd. as substances with possible cytokinin activity.

L6 ANSWER 34 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 39639-52-6 REGISTRY

CN 1H-Purine-2,6-diamine, N6-(4-nitrophenyl)-N2-(phenylmethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H15 N7 O2

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 78:16123 Synthesis and study of 2,6-diaminopurines. Tret'yakova, G. S.; Nedel'kina, N. N.; Cherkasov, V. M. (Inst. Org. Khim.,

Kiev, USSR). Ukr. Khim. Zh. (Russ. Ed.), 38(6), 602-5 (Russian) 1972. CODEN: UKZHAU.

AB 2,6-Dichloropurine was treated with cyclohexyl-, admantyl-, and benzylamines, and with morpholine, p-toluidine, and p-nitroaniline to replace the Cl atom in position 2. By use of more amine, disubstituted compds. were obtained using morpholine, benzylamine, and p-toluidine.

The

Me,

Cl atom of 6-chloro-2-benzylaminopurine was replaced by p-XC6H4NH (X = $^{\circ}$

NO2) and the Cl of 6-chloro-2-cyclohexylaminopurine was replaced with p-O2NC6H4NH. These compds. were prepd. as substances with possible cytokinin activity.

L6 ANSWER 35 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 39639-51-5 REGISTRY

CN 1H-Purine-2,6-diamine, N2-cyclohexyl-N6-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C17 H19 N7 O2

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 78:16123 Synthesis and study of 2,6-diaminopurines. Tret'yakova, G. S.; Nedel'kina, N. N.; Cherkasov, V. M. (Inst. Org. Khim.,

Kiev, USSR). Ukr. Khim. Zh. (Russ. Ed.), 38(6), 602-5 (Russian) 1972. CODEN: UKZHAU.

AB 2,6-Dichloropurine was treated with cyclohexyl-, admantyl-, and benzylamines, and with morpholine, p-toluidine, and p-nitroaniline to replace the Cl atom in position 2. By use of more amine, disubstituted compds. were obtained using morpholine, benzylamine, and p-toluidine.

The Me,

Cl atom of 6-chloro-2-benzylaminopurine was replaced by p-XC6H4NH (X = $\frac{1}{2}$

NO2) and the Cl of 6-chloro-2-cyclohexylaminopurine was replaced with p-O2NC6H4NH. These compds. were prepd. as substances with possible cytokinin activity.

L6 ANSWER 36 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 39639-50-4 REGISTRY

CN 1H-Purin-6-amine, 2-chloro-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C11 H7 C1 N6 O2

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 127:34237 Preparation of purine derivatives. Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal (Novartis Ag,

Switz.; Zimmermann, Juerg; Capraro, Hans-Georg; Peterli, Patricia; Furet, Pascal). PCT Int. Appl. WO 9716452 A1 19970509, 97 pp. DESIGNATED STATES: W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP4573 19961022. PRIORITY: CH 1995-3094 19951101;

CH 1996-2213 19960910.

GI

The

$$Rq$$
 $NR1$
 R^2m
 R^3R^4N
 R^2n
 R^2n

AB 2-Amino-6-anilino-purine derivs. I (R = halo, alkyl, HO, alkanoyloxy, alkoxy, substituted alkoxy, carboxyl, alkoxycarbonyl, carbamoyl, amino, aminosulfonyl, F3C; R1 = H, carbamoyl, alkylcarbamoyl; R2 = alkyl, Ph, substituted Ph; R3 = H, amino, phenylamino, alkylamino, HO, phenoxy, alkoxy, acyl, carbocyclic radical, or heterocyclic radical; R4 = amino, OH, phenoxy, alkoxy, acyl, substituted hydrocarbon radical, carbocyclic radical, or heterocyclic radical; R3R4 may form a ring; m and n are 0, 1; q = 1-5) were prepd. These compds. inhibit p34cdc2/cyclin Bcdc13 kinase and can be used for treatment of hyperproliferative diseases, for example tumor diseases (no data). Thus,

2-chloro-6-(3-chlorophenylamino)-9-ethyl-

9H-purine, prepd. in two steps from 3-chloroaniline and 2,6-dichloropurine, was treated with ethylenediamine to give 2-(2-aminoethylamino)-6-(3-chlorophenylamino)-9-ethyl-9H-purine.

REFERENCE 2: 78:16123 Synthesis and study of 2,6-diaminopurines. Tret'yakova, G. S.; Nedel'kina, N. N.; Cherkasov, V. M. (Inst. Org. Khim.,

Kiev, USSR). Ukr. Khim. Zh. (Russ. Ed.), 38(6), 602-5 (Russian) 1972. CODEN: UKZHAU.

AΒ 2,6-Dichloropurine was treated with cyclohexyl-, admantyl-, and benzylamines, and with morpholine, p-toluidine, and p-nitroaniline to replace the Cl atom in position 2. By use of more amine, disubstituted compds. were obtained using morpholine, benzylamine, and p-toluidine.

Cl atom of 6-chloro-2-benzylaminopurine was replaced by p-XC6H4NH (X = Me,

NO2) and the Cl of 6-chloro-2-cyclohexylaminopurine was replaced with p-O2NC6H4NH. These compds. were prepd. as substances with possible cytokinin activity.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 78:16123 Synthesis and study of 2,6-diaminopurines. Tret'yakova, G. S.; Nedel'kina, N. N.; Cherkasov, V. M. (Inst. Org. Khim.,

Kiev, USSR). Ukr. Khim. Zh. (Russ. Ed.), 38(6), 602-5 (Russian) 1972. CODEN: UKZHAU.

AB 2,6-Dichloropurine was treated with cyclohexyl-, admantyl-, and benzylamines, and with morpholine, p-toluidine, and p-nitroaniline to replace the Cl atom in position 2. By use of more amine, disubstituted compds. were obtained using morpholine, benzylamine, and p-toluidine.

The

Cl atom of 6-chloro-2-benzylaminopurine was replaced by p-XC6H4NH (X = Me,

NO2) and the Cl of 6-chloro-2-cyclohexylaminopurine was replaced with p-O2NC6H4NH. These compds. were prepd. as substances with possible cytokinin activity.

L6 ANSWER 38 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 16124-77-9 REGISTRY

CN Purine, 2-chloro-6-[.beta.-(diethylamino)-p-phenetidino]- (8CI) (CA INDEX

NAME)

FS 3D CONCORD

MF C17 H21 C1 N6 O

LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXLIT (*File contains numerically searchable property data)

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 67:99762 Nonsteroidal hypocholesteremic agents. I. Synthesis and serum sterol lowering properties of substituted 4-(2-dialkylaminoethoxy)diphenylamines and related compounds. Bach, Frederick L., Jr.; Barclay, John C.; Cohen, Elliott (American Cyanamid Co., Pearl River, N. Y., USA). J. Med. Chem., 10(5), 802-6 (English) 1967. CODEN: JMCMAR.

GI For diagram(s), see printed CA Issue.

AB The prepn. and serum sterol lowering properties of a series of 4,4'-disubstituted diphenylamines and related compds., e.g. I, are discussed. Initial screening data indicate that several of these compds.,

synthesized by conventional means, possess oral activity greater than most

nonsteroidal hypocholesteremic agents reported to date.

L6 ANSWER 39 OF 39 REGISTRY COPYRIGHT 2000 ACS

RN 14051-72-0 REGISTRY

CN 1H-Purine-2,6-diamine, N6-phenyl- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Purine, 2-amino-6-anilino- (6CI, 8CI)

OTHER NAMES:

CN 2-Amino-6-(phenylamino)purine

CN 2-Amino-6-anilinopurine

FS 3D CONCORD

MF C11 H10 N6

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, TOXLIT, USPATFULL (*File contains numerically searchable property data)

6 REFERENCES IN FILE CA (1967 TO DATE)

6 REFERENCES IN FILE CAPLUS (1967 TO DATE)

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 126:131752 Preparation of phosphonate acyclic nucleotide

derivatives as antiviral agents. Ubasawa, Masaru; Takashima, Hideaki; Sekiya, Kouichi; Inoue, Naoko; Yuasa, Satoshi; Kamiya, Naohiro (Mistubishi

Chemical Corporation, Japan; Ubasawa, Masaru; Takashima, Hideaki; Sekiya, Kouichi; Inoue, Naoko; Yuasa, Satoshi; Kamiya, Naohiro). PCT Int. Appl. WO 9700262 Al 19970103, 58 pp. DESIGNATED STATES: W: CA, CN, JP, KR, US;

RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (Japanese). CODEN: PIXXD2. APPLICATION: WO 1996-JP1631 19960614. PRIORITY: JP 1995-149014 19950615.

GΙ

AB Compds. represented by general formula (I; R1 = H, C1-6 alkyl or C7-10 aralkyl; R2 = C1-6 alkyl, C7-10 aralkyl or phenyl; R3, R4 = H, C1-6 alkyl,

acyloxymethyl, acylthioethyl, ${\tt Et}$ substituted by at least one halogen atom;

R5 = H, C1-4 alkyl, C1-4 hydroxyalkyl, C1-4 alkyl substituted by at least one halogen atom; X = C or N), which show antiviral activity with high oral absorbability, are prepd. Thus, 2-amino-6-(dimethylamino)purine was suspended in DMSO and reacted with 1,8-diazabicyclo[5.4.0]undec-7-ene at 100.degree. for 1 h, followed by adding 2-[bis(2,2,2-trifluoreethyl)phosphorylmethogylethyl indide and the resulting mint

trifluoroethyl)phosphonylmethoxy]ethyl iodide, and the resulting mixt.

was

allowed to react at 100.degree. for 2 h to give 12% 2,6-diamino-9- [(phosphonomethoxy)ethyl]purine I (R1 = R2 = Me, R3 = R4 = CF3CH2, R5 = $\frac{1}{2}$

Н,

X = C). This compd. in vitro inhibited 92 and 100% at 1 and 100 .mu.M, resp., the synthesis of DNA synthesis of hepatitis B virus in HB611 cells and showed 50% cell toxicity for HB611 cell at >1,000 .mu.M.

REFERENCE 2: 120:217083 The mass spectrometry of 2-amino-6-arylaminopurines.

Yakout, E. M. A. (Dep. Pesticide Chem., Natl. Res. Cent., Cairo, Egypt).
Bull. Natl. Res. Cent. (Egypt), 18(1), 11-17 (English) 1993. CODEN:
BNRCET.

AB Principal modes of fragmentation of the title spectra under electron impact were detd.

REFERENCE 3: 120:29465 Preparation of (2',3'-dideoxy-3'-.beta.-D-erythropentofuranosyl)-9H-purines as antiviral nucleosides. Burns, Charlene Louise; Koszalka, George Walter; Krenitsky, Thomas Anthony (Wellcome Foundation Ltd., UK). PCT Int. Appl. WO 9314103 A1 19930722, 94

pp. DESIGNATED STATES: RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1993-GB4 19930105. PRIORITY:

AB Title compds. I [R1 = H, amino, halo; R2 = halo; NR4R5, R4, R5 = H, C1-4 hydroxyalkyl, C1-6 alkyl, C3-6 cycloalkyl, C2-6 alkenyl, C6-10 aryl, (un)substituted C6-10arylC1-3alkyl, etc.; R6O(Ar)(CH2)n (R6 = C1-6 alkyl, Ar = C6-10 aryl, n = 0-3); R4R5 = N of a 3 to 7-membered heterocyclic

ring

optionally contg. 1 or more other hetero atoms selected from O, N, S; S(O) nR7, n = 0-2, R7 = C1-6 alkyl, C3-6 cycloalkyl, etc.; OR8, OR8, OR8 = H, OR8 cycloalkyl, OR8 cycloalkyl, etc.; OR8 = H, amino, halo, OR8 = H, OR8 cycloalkyl, etc.; OR8 = H, amino, halo, OR8 = H, OR8 cycloalkyl, etc.; OR8 = H, amino, halo, OR8 = H, OR8 cycloalkyl, etc.; OR8 = H, amino, halo, OR8 = H, OR8 cycloalkyl, etc.; OR8 = H, amino, halo, OR8 = H, OR8 = H, amino, halo, OR8 = H, OR8 = H, amino, halo, OR8 = H, amino, halo, OR8 = H, OR8 = H, amino, halo, OR8 = H, a

on

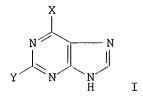
DEAE cellulose to give 26% I (R1 = NH2, R2 = Me2N, R3 = H) (II). II showed an IC50 = 8.mu.M against HIV in MT4 cells. Various formulations for I are also reported.

REFERENCE 4: 110:172972 Phosphorus pentoxide in organic synthesis. XXXVII. Synthesis of 2-amino-6-arylaminopurines. Yakout, El Sayed M. A.; Soe, Henrik M.; Pedersen, Erik B. (Dep. Chem., Odense Univ., Odense, DK-5230, Den.). Acta Chem. Scand., Ser. B, B42(4), 257-8 (English) 1988. CODEN: ACBOCV. ISSN: 0302-4369.

GΙ

AB Aminopurines I (R = Ph, substituted Ph) were obtained in 45-90% yield by heating guanine with RNH2.HCl in the presence of P2O5 and Et3N.HCl.

REFERENCE 5: 107:31115 Silver halide photographic material. Sakamoto, Hidekazu; Kaneko, Yutaka (Konishiroku Photo Industry Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 61256346 A2 19861113 Showa, 17 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1985-99251 19850510.



AB A Ag halide photog. material contains .gtoreq.1 pyrimidoimidazole deriv. of the formula I [X = NR1R2, NHCZR3, NHSO2R4 (R1, R2 = H, alkyl, aryl; R3 = alkyl, aryl, amino; R4 = alkyl, aryl; Z = O, S); Y = H, OH, NH2] as a fog inhibitor. Fog formation is suppressed even on extended storage.

REFERENCE 6: 67:73588 Irreversible enzyme inhibitors. XCII. Inhibition of xanthine oxidase by some purines and pyrimidines. Baker, Bernard Randall;

Hendrickson, J. L. (Univ. of California, Santa Barbara, CA, USA). J. Pharm. Sci., 56(8), 955-9 (English) 1967. CODEN: JPMSAE.

Twenty-six compds. were investigated as inhibitors of xanthine oxidase, the enxyme that can also detoxify 6-mercaptopurine; these compds. consisted of 19 purines, 4 pyrimidines, 2 8-azapurines, and 1 imidazole. Among the inhibitors that complexed to xanthine oxidase as well or better than the substrate, hypoxanthine, were thioguanine, adenine, and 6,8-dihydroxy-2-methylthiopurine (I). The larger 2-benzylthio-6,8-dihydroxypurine (II) was synthesized and inhibited equally as well as I. 2-Benzylthiohypoxanthine (III) and 8-benzylthiohypoxanthine (IV) were synthesized; these compds. complexed 11-fold and 2-fold better, resp., to the enzyme than did the substrate. Thus, the enzyme showed bulk tolerance

for the benzylthio group of II-IV; the benzylthio group is a local group for placement of electrophilic groups to give candidate active-site-directed irreversible inhibitors of xanthine oxidase. 33 references.

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ANSWER 1 OF 1 CAOLD COPYRIGHT 2000 ACS L7 ΑN CA54:6747a CAOLD potential purine antagonists - (XIX) synthesis of some ΤI 9-alkyl(aryl)-2-amino-6-substituted purines and related v-triazolo[d]pyrimidines Koppel, Henry C.; O'Brien, D. E.; Robins, R. K. ΑU ΙT 2239-25-0 2879-14-3 5444-47-3 5472-85-5 6318-28-1 .7780-34-9 14051-72-0 14443-33-5 14443-34-6 14937-64-5 14937-72-5 14937-71-4 14937-73-6 14937-74-7 15065-50-6 17419-08-8 17756-37-5 17756-35-3 19188-48-8 21318-84-3 30412-45-4 30546-08-8 34396-82-2 40769-49-1 33359-01-2 49753-53-9 61971-98-0 64414-74-0 92723-90-5 93692-99-0 99421-31-5 91183-14-1 99851-86-2 99973-83-8 101134-16-1 101352-54-9 107892-35-3 108776-70-1 108870-41-3 99852-37-6 109221-75-2 109508-08-9 109842-62-8 110062-34-5 110334-53-7 110394-88-2 114166-07-3 114329-01-0 114352-23-7 114352-57-7 115984-55-9 120614-08-6 121791-15-9 131240-35-2 132105-55-6 132129-43-2

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